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THE NUMERICAL CALCULATION OF TRAVELING WAVE SOLUTIONS  
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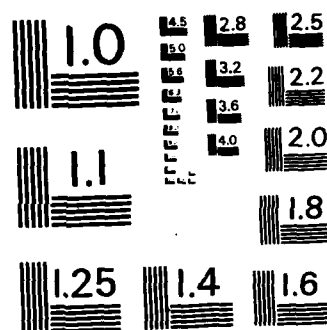
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THE NUMERICAL CALCULATION OF TRAVELING  
WAVE SOLUTIONS OF NONLINEAR PARABOLIC  
EQUATIONS ON THE LINE

Thomas Hagstrom and H. B. Keller

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**Mathematics Research Center  
University of Wisconsin—Madison  
610 Walnut Street  
Madison, Wisconsin 53705**

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THE NUMERICAL CALCULATION OF TRAVELING WAVE SOLUTIONS  
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ABSTRACT

✓ The long time behavior of the solutions of nonlinear parabolic initial value problems on the line has been investigated by many authors. In particular they have shown, under certain assumptions, the existence of traveling waves to which a large class of initial data eventually evolves. They have also proved that which traveling wave solution is picked out as the asymptotic state often depends on the behavior of the initial data at infinity. This causes difficulties for the numerical simulation of the long time evolution of such problems. In particular, if an artificial boundary is introduced, the boundary condition imposed there must depend on the initial data in the discarded region. In this work we derive such boundary conditions, based on the Laplace transform solution of the linearized problems at  $\infty$ . We illustrate their utility by presenting a numerical solution of Fisher's equation, a nonlinear parabolic equation with traveling wave solutions which has been proposed as a model in genetics.

AMS (MOS) Subject Classifications: 65M99, 35K15

Key Words: Artificial boundary conditions, parabolic traveling waves

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\*Department of Applied Mathematics, California Institute of Technology,  
Pasadena, CA 91125

## SIGNIFICANCE AND EXPLANATION

Nonlinear partial differential equations of parabolic type arise in various applications. Examples include models of chemical kinetics and population dynamics. In many cases it is the evolution of the initial data into some simple final state which is of interest. For a class of initial value problems on the line, other authors have shown that the final state is usually a traveling wave and is determined by the initial data at infinity. In this work we present a method for the numerical simulation of this evolution.

As a finite domain is required for the numerical method, it is necessary to introduce artificial boundaries. The boundary conditions imposed there must depend on the initial data in the discarded regions if the correct long time solution is to be found. We construct such conditions using the Laplace transform solution of the linearized problems at  $t = \infty$ . Their utility is illustrated by the solution of Fisher's equation, a model of the spatial advance of an advantageous gene. It is hoped that this method will give reliable results when applied to problems whose final state is not known beforehand.



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THE NUMERICAL CALCULATION OF TRAVELING WAVE SOLUTIONS  
OF NONLINEAR PARABOLIC EQUATIONS ON THE LINE

Thomas Hagstrom and H. B. Keller\*

1 INTRODUCTION

We consider the numerical solution of the Cauchy problem for a class of nonlinear parabolic equations;

$$(1.1) \quad \begin{aligned} & a) \quad u_t = f(u_{xx}, u_x, u), \quad -\infty < x < \infty, \quad t > 0; \\ & b) \quad \lim_{x \rightarrow \infty} u(x, t) = \phi_+, \quad \lim_{x \rightarrow -\infty} u(x, t) = \phi_-; \\ & c) \quad u(x, 0) = u_0(x); \\ & d) \quad \frac{\partial}{\partial a} f(a, b, c) > 1 \quad \text{for all } a, b, c. \end{aligned}$$

We assume that  $\phi_{\pm}$  satisfy:

$$(1.2) \quad \begin{aligned} & f(0, 0, \phi_{\pm}) = 0; \\ & f_u(0, 0, \phi_{\pm}) \neq 0, \end{aligned}$$

and that the initial data,  $u_0(x)$ , satisfies (1.1b). In particular, we are interested in simulating the evolution of the initial data into traveling waves.

Hagan [3,4] has presented an extensive analysis of problem (1.1). We paraphrase some of his results below:

- (i) Nonmonotonic waves are unstable in general.
- (ii) The stability of monotonic waves of speed  $c$  can, in general, be determined by an examination of their trajectories in the phase plane of:

$$(1.3) \quad \begin{aligned} & w' = v; \\ & f(v', v, w) + cv = 0. \end{aligned}$$

- (iii) If traveling waves exist, a large class of initial data satisfying (1.1b) will evolve to a traveling wave.

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\*Department of Applied Mathematics, California Institute of Technology, Pasadena, CA 91125

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(iv) In certain situations, infinitely many wavespeeds,  $c$ , are allowed. In this case, the traveling wave which is eventually seen depends on the behavior of the initial data at infinity.

The numerical solution of (1.1) requires a finite computational domain. One way to obtain such a domain is to introduce artificial boundaries at the points

$x = \tau_{\pm}$ ,  $\tau_{+} > \tau_{-}$ , and impose boundary conditions there. The derivation of proper boundary conditions is the main subject of this work. A general theory of boundary conditions at an artificial boundary is given by the authors in [6]. This theory is not directly applicable to time dependent problems in unbounded spatial domains such as (1.1). However, a Laplace transformation in time yields a problem of the right form. In section 2, conditions are derived for the transformed problem and inverted to yield conditions in the real variables.

We note that use of the proper boundary conditions is crucial whenever (iv) holds. Then, the "naive" conditions:

$$(1.4) \quad \begin{aligned} u(\tau_{+}, t) &= \phi_{+}, \\ U(\tau_{-}, t) &= \phi_{-}, \end{aligned}$$

must, in general, fail to lead to the correct long time solution.

In section 3 a specific problem of the form (1.1) is introduced: the Cauchy problem for Fisher's equation. It has traveling wave solutions of all speeds  $c > 2$ . Gazdag and Canosa [1] present a numerical solution of Fisher's equation using boundary conditions analogous to (1.4). As predicted by the theory, their solution always evolved to the traveling wave of minimum speed. Here we present calculations using the boundary conditions derived in section 2. The numerical solution is seen to evolve to the correct traveling wave for a variety of choices of initial data.

We note that the method of deriving boundary conditions presented here can be applied to other time dependent problems, including some problems of hyperbolic type. For other examples the reader is referred to Gustafsson and Kreiss [2] and Hagstrom [5].

The authors thank Prof. J. D. Murray for bringing this problem to their attention.

## 2. CONSTRUCTION OF THE BOUNDARY CONDITIONS

We now construct boundary conditions at the right boundary,  $x = \tau_+$ . (The construction at the left will be analogous.) Only the linearized problem in the tail is considered and a coordinate system moving to the right with speed  $c$  is assumed;

$$(2.1) \quad \begin{aligned} a) \quad & v(x, t) = u(x, t) - \phi_+, \quad x > \tau_+; \\ b) \quad & v_t = f_1 v_{xx} + f_2 v_x + cv_x + f_3 v; \\ c) \quad & v(x, 0) = u_0(x) - \phi_+; \\ d) \quad & \lim_{x \rightarrow \infty} v(x, t) = 0; \end{aligned}$$

where the constants  $f_i$  are given by:

$$(2.2) \quad \begin{aligned} f_1 &= \frac{\partial f}{\partial (u_{xx})} (0, 0, \phi_+); \\ f_2 &= \frac{\partial f}{\partial (u_x)} (0, 0, \phi_+); \\ f_3 &= \frac{\partial f}{\partial u} (0, 0, \phi_+). \end{aligned}$$

Following the general ideas presented by the authors in [6], two problems must be solved; boundary conditions for the homogeneous problem, (2.1b,d) combined with zero initial data, must be found as well as a particular solution of (2.1b,d) which satisfies (2.1c). The homogeneous problem is considered first.

### Boundary Conditions for the Homogeneous Problem

We introduce the temporal Laplace transform:

$$\hat{\omega}(x, s) = \int_0^{\infty} e^{-st} \omega(x, t) dt.$$

If  $\omega$  is a solution of (2.1b,d) with zero initial data, then  $\hat{\omega}$  satisfies:

$$(2.3) \quad \begin{aligned} f_1 \hat{\omega}_{xx} + (f_2 + c) \hat{\omega}_x + (f_3 - s) \hat{\omega} &= 0; \\ \lim_{x \rightarrow \infty} \hat{\omega}(x, s) &= 0. \end{aligned}$$

Equation (2.3a) has the basic exponential solutions:



$$(2.4) \quad \hat{\omega} = e^{\pm k_{\pm}(s;c)x},$$

where  $k_{\pm}(s;c)$  are given by:

$$(2.5) \quad k_{\pm} = \frac{-(f_2 + c)}{2f_1} \pm \frac{1}{2f_1} [(f_2 + c)^2 + 4f_1(s - f_3)]^{1/2}.$$

For real part of  $s$  sufficiently large,  $k_+$  will have real part positive and  $k_-$  will have real part negative. (Recall,  $f_1 > 1$ .) Hence, the admissible solution has exponent  $k_-$ . It satisfies:

$$(2.6) \quad \hat{\omega}_x(\tau_+, s) = k_-(s;c) \hat{\omega}(\tau_+, s);$$

which can be rewritten;

$$\frac{\hat{\omega}_x(\tau_+, s)}{k_-(s;c)} = \hat{\omega}(\tau_+, s).$$

Using the convolution formulas and the expression for the inverse transform of  $\frac{1}{k_-}$  (see, e.g., Oberhettinger and Badii [8]), (2.7) can be expressed in the real variables:

$$(2.8) \quad -\sqrt{f_1} \int_0^t e^{[f_3 - \alpha^2](t-p)} \left[ \frac{1}{\sqrt{\pi(t-p)}} - \alpha e^{\alpha^2(t-p)} \text{Erfc}(\alpha\sqrt{t-p}) \right] \omega_x(\tau_+, p) dp = \omega(\tau_+, t);$$

$$\alpha \equiv \frac{f_2 + c}{2\sqrt{f_1}}.$$

#### Particular Solution

We now find particular solutions, assuming that  $u_0 - \phi_+$  can be expressed as a finite sum of exponentials:

$$u_0(x) - \phi_+ = \sum_{j=1}^N d_j e^{-\alpha_j(x-\tau_+)}, \quad \alpha_j > 0, \quad x > \tau_+.$$

We note from Hagan's analysis [3] it is necessary in many cases that  $u_0 - \phi_+$  decay at least exponentially if traveling wave solutions are to be found. From (2.5), with

$s = 0$ , we see that traveling waves of speed  $c$  have exponential decay rates given by:

$$(2.9) \quad g_{\pm}(c) = -\frac{f_2 + c}{2f_1} \pm \frac{1}{2f_1} [(f_2 + c)^2 - 4f_1 f_3]^{1/2}.$$

From (2.9) we see that given any exponent,  $-\alpha_j$ , there exists a unique speed  $c_j$  such that:

$$(2.10) \quad -\alpha_j = g_-(c_j) \quad \text{or} \quad -\alpha_j = g_+(c_j).$$

It is given by:

$$(2.11) \quad c_j = \frac{f_3}{\alpha_j} + f_1 \alpha_j - f_2.$$

Hence, each exponential can be associated with a unique traveling wave solution, from which a particular solution can be found:

$$(2.12) \quad v_p(x, t) = \sum_{j=1}^N d_j e^{\alpha_j \tau_+} e^{-\alpha_j (x - (c_j - c)t)}.$$

Combining (2.8) and (2.12) yields the following linearized boundary condition for  $u$  at  $x = \tau_+$ :

$$(2.13) \quad -\sqrt{f_1} \int_0^t e^{[f_3 - \alpha^2](t-p)} \left[ \frac{1}{\sqrt{\pi(t-p)}} - \alpha e^{\alpha^2(t-p)} \operatorname{Erfc}(\alpha\sqrt{t-p}) \right] (u_x(\tau_+, p) + \sum_{j=1}^N \alpha_j d_j e^{\alpha_j (c_j - c)p}) dp \\ = u(\tau_+, t) - \phi_+ - \sum_{j=1}^N d_j e^{\alpha_j (c_j - c)t},$$

where

$$(2.14) \quad \begin{aligned} \text{a) } \alpha &= \frac{f_2 + c}{2\sqrt{f_1}}; \\ \text{b) } u_0(x) &= \phi_+ + \sum_{j=1}^N d_j e^{-\alpha_j (x - \tau_+)}, \quad x > \tau_+. \end{aligned}$$

#### Conditions at the Left Boundary

A similar boundary condition can be derived at the left boundary,  $x = \tau_-$ . In transform variables, a solution to the linearized, homogeneous problem on  $(-\infty, \tau_-]$  must

satisfy:

$$(2.15) \quad \frac{\hat{\omega}_x(\tau_-, s)}{\bar{k}_+(s; c)} = \hat{\omega}(\tau_-, s),$$

where

$$(2.16) \quad \bar{k}_+ = \frac{-(\bar{f}_2 + c)}{2\bar{f}_1} + \frac{1}{2\bar{f}_1} [(\bar{f}_2 + c)^2 + 4\bar{f}_1(s - \bar{f}_3)]^{1/2}.$$

We now have:

$$(2.17) \quad \begin{aligned} \bar{f}_1 &= \frac{\partial f}{\partial (u_{xx})} (0, 0, \phi_-); \\ \bar{f}_2 &= \frac{\partial f}{\partial (u_x)} (0, 0, \phi_-); \\ \bar{f}_3 &= \frac{\partial f}{\partial u} (0, 0, \phi_-). \end{aligned}$$

The inverse transform of (2.15) is given by:

$$(2.18) \quad \sqrt{\bar{f}_1} \int_0^t e^{(\bar{f}_3 - \bar{a}^2)(t-p)} \left[ \frac{1}{\sqrt{\pi(t-p)}} + \bar{a} e^{\bar{a}^2(t-p)} \operatorname{Erfc}(-\bar{a}\sqrt{t-p}) \right] \omega_x(\tau_-, p) dp = \omega(\tau_-, t);$$

$$\bar{a} = \frac{\bar{f}_2 + c}{2\sqrt{\bar{f}_1}}.$$

To find a particular solution we assume that

$$u_0(x) - \phi_- = \sum_{j=1}^M \bar{a}_j e^{\bar{a}_j(x - \tau_-)}, \quad \bar{a}_j > 0, \quad x < \tau_-.$$

Each exponent,  $\bar{a}_j$ , can be uniquely associated with a linear traveling wave of speed  $\bar{c}_j$  through equation (2.16) (with  $s = 0$ ):

$$(2.19) \quad \bar{c}_j = -\bar{f}_2 - \bar{f}_1 \bar{a}_j - \frac{\bar{f}_3}{\bar{a}_j},$$

leading to the particular solution:

$$(2.20) \quad \bar{v}_p(x, t) = \phi_- + \sum_{j=1}^M \bar{d}_j e^{-\bar{\alpha}_j \tau_-} \bar{\alpha}_j^{(x + (c - \bar{c}_j)t)}$$

Combining (2.20) with (2.18) yields a linear boundary condition at  $\tau_-$ , analogous to (2.13);

$$(2.21) \quad \sqrt{\bar{f}_1} \int_0^t e^{[\bar{f}_3 - \bar{\alpha}^2](t-p)} \left[ \frac{1}{\sqrt{\pi(t-p)}} + \bar{\alpha} e^{\bar{\alpha}^2(t-p)} \operatorname{Erfc}(-\bar{\alpha}\sqrt{t-p}) \right] (u_x(\tau_-, p) - \sum_{j=1}^M \bar{\alpha}_j \bar{d}_j e^{\bar{\alpha}_j(c - \bar{c}_j)p}) dp \\ = u(\tau_-, t) - \phi_- - \sum_{j=1}^M \bar{d}_j e^{\bar{\alpha}_j(c - \bar{c}_j)t};$$

where

$$(2.22) \quad \text{a) } \bar{\alpha} = \frac{\bar{f}_2 + c}{2\sqrt{\bar{f}_1}};$$

$$\text{b) } u_0(x) = \phi_- + \sum_{j=1}^M \bar{d}_j e^{\bar{\alpha}_j(x - \tau_-)}, \quad x < \tau_-.$$

### 3. Application to Fisher's Equation

We now apply the results of preceding section to Fisher's equation:

$$(3.1) \quad \begin{aligned} \text{a) } u_t &= u_{xx} + u(1 - u), \quad x \in (-\infty, \infty), \quad t > 0; \\ \text{b) } \lim_{x \rightarrow \infty} u(x, t) &= 0, \quad \lim_{x \rightarrow -\infty} u(x, t) = 1; \\ \text{c) } u(x, 0) &= u_0(x). \end{aligned}$$

Problem (3.1) has arisen as a model of the propagation of an advantageous gene. For a discussion of this application see, for example, Moran [7]. It is a special case of (1.1) and various statements concerning the behavior of its solution are consequences of Hagan's [3] general analysis:

- (i) There exist traveling wave solutions of all wavespeeds  $c > 2$ .

(ii) All positive initial data,  $u_0(x)$ , decaying at least exponentially as  $x \rightarrow \infty$  evolves to a unique traveling wave.

(iii) If  $u_0(x) \sim e^{-\beta x}$  as  $x \rightarrow \infty$  then the solution evolves to a wave of speed  $c(\beta)$  given by:

$$(3.2) \quad c(\beta) = \begin{cases} \frac{1 + \beta^2}{\beta}, & \beta < 1 \\ 2 & \beta > 1. \end{cases}$$

The linearized boundary conditions, (2.13) and (2.21), are easily specialized to this problem. As in section 2, we introduce a coordinate system moving to the right with speed  $c$  and choose  $\tau_+$  and  $\tau_-$  as our artificial boundary locations. We assume  $u_0(x)$  can be represented as a finite sum of exponentials in the tails:

$$(3.3) \quad u_0(x) = \sum_{j=1}^N d_j e^{-\alpha_j(x-\tau_+)}, \quad x > \tau_+;$$

$$u_0(x) = \sum_{j=1}^M \bar{d}_j e^{-\bar{\alpha}_j(x-\tau_-)} + 1, \quad x < \tau_-.$$

The boundary conditions we impose are:

$$(3.4) \quad \begin{aligned} \text{a) } & \int_0^t e^{-\left(1 + \frac{c^2}{4}\right)(t-p)} \left[ \frac{1}{\sqrt{\pi(t-p)}} - \frac{c}{2} e^{\frac{c^2}{4}(t-p)} \operatorname{Erfc}\left(\frac{c}{2}\sqrt{t-p}\right) \right] (u_x(\tau_+, p) + \sum_{j=1}^N \alpha_j d_j e^{(1+\alpha_j^2-\alpha_j c)p}) dp \\ & = u(\tau_+, t) - \sum_{j=1}^N d_j e^{(1+\alpha_j^2-\alpha_j c)t}, \\ \text{b) } & \int_0^t e^{-\left(1 + \frac{c^2}{4}\right)(t-p)} \left[ \frac{1}{\sqrt{\pi(t-p)}} + \frac{c}{2} e^{\frac{c^2}{4}(t-p)} \operatorname{Erfc}\left(-\frac{c}{2}\sqrt{t-p}\right) \right] (u_x(\tau_-, p) - \sum_{j=1}^M \bar{\alpha}_j \bar{d}_j e^{(\bar{\alpha}_j^2+\bar{\alpha}_j c-1)p}) dp \\ & = u(\tau_-, t) - 1 - \sum_{j=1}^M \bar{d}_j e^{(\bar{\alpha}_j^2+\bar{\alpha}_j c-1)t}. \end{aligned}$$

We note that, by (3.3), the true solution should evolve to a wave of speed  $c(\beta)$  given by (3.2) where

$$(3.5) \quad \beta = \min_j \{\alpha_j\}.$$

In certain circumstances the particular terms in (3.4a) have a large exponential growth in time. As this could be a source of error in a numerical computation, the integrals involving them were done exactly. This allows us to rewrite the right boundary condition:

$$(3.4a') \quad \begin{aligned} & - \int_0^t e^{-\frac{c^2}{4}(t-p)} \left[ \frac{1}{\sqrt{\pi(t-p)}} - \frac{c}{2} e^{\frac{c^2}{4}(t-p)} \operatorname{Erfc}\left(\frac{c}{2} \sqrt{t-p}\right) \right] u_x(\tau_+, p) dp \\ & = u(\tau_+, t) + \sum_{j=1}^N f_j(t), \end{aligned}$$

where

$$(3.6) \quad \begin{aligned} f_j(t) &= \alpha_j d_j \left[ \frac{-c}{2(1-k_j)} e^t \operatorname{Erfc}\left(\frac{c}{2} \sqrt{t}\right) + \frac{\left[k_j + \frac{c^2}{4} - 1\right]^{1/2}}{(1-k_j)} e^{k_j t} \operatorname{Erfc}\left(\sqrt{\left(k_j + \frac{c^2}{4} - 1\right)t}\right) + h_j(t) \right]; \\ h_j(t) &= \begin{cases} 0, & \alpha_j = \frac{c}{2} + \sqrt{\frac{c^2}{4} + k_j - 1} \\ -2 \frac{\sqrt{\frac{c^2}{4} + k_j - 1}}{(1-k_j)} e^{k_j t}, & \alpha_j = \frac{c}{2} - \sqrt{\frac{c^2}{4} + k_j - 1}; \end{cases} \\ k_j &= 1 + \alpha_j^2 - \alpha_j c. \end{aligned}$$

We note that (3.4a') explicitly contains the different evolution of initial data with large and small decay rates.

Presented below are the results of some numerical computations of solutions of (3.1) using the boundary conditions (3.4a',b). A uniform grid was introduced and spatial derivatives were replaced by centered finite differences. The method was implicit in time and stable for the ratio of the time step to the grid size sufficiently small. At each step a nonlinear system of equations was solved using Newton's method with an explicit step

taken to generate the initial guess. The boundaries were located midway between gridpoints and the integrals there were approximated by the trapezoid rule (away from the singularity). For all cases described below the grid ranged between -12 and 12 and contained 171 points. The time step is .025, well within the stable region in all cases. Initial conditions were generated in the following way: expansions in the tail, (3.3), were input and smoothly connected (two continuous derivatives) by a combination of polynomial and exponential functions. The computations shown were performed on a VAX 11/780 at the University of Wisconsin at Madison, though others were done on the IBM 4341 of the Applied Mathematics Department at the California Institute of Technology.

Figure 1 shows the evolution, in a coordinate system moving with speed 4, of initial data which decays, at both  $t=0$ , at a rate compatible with a wave of speed 4. The initial data and solutions at intervals of 25 time steps are displayed. A steady state is reached which must be moving with speed 4. Figure 2 contains the final state (solid line) of Figure 1. This is the solution at  $t = 6.875$ . Plotted with it is a wave of speed 4 found by a finite difference solution of the relevant steady problem. The agreement between the two solutions is seen to be excellent.

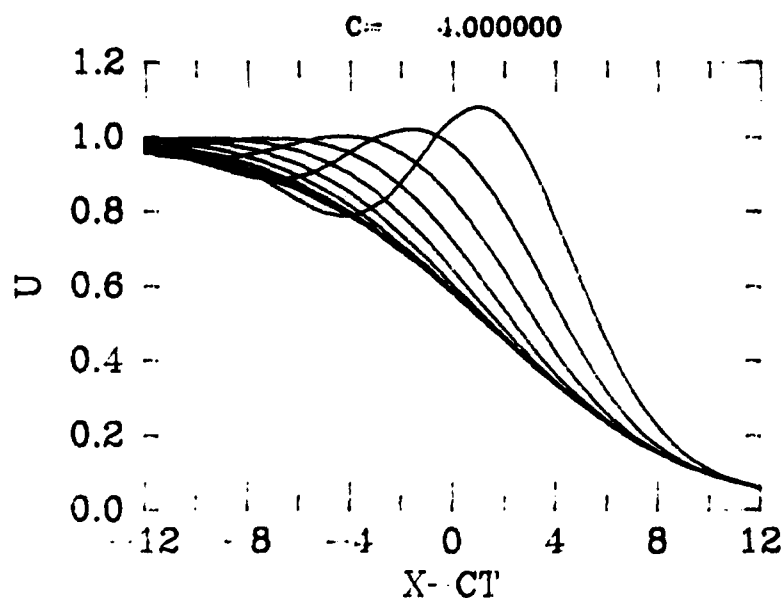


Figure 1

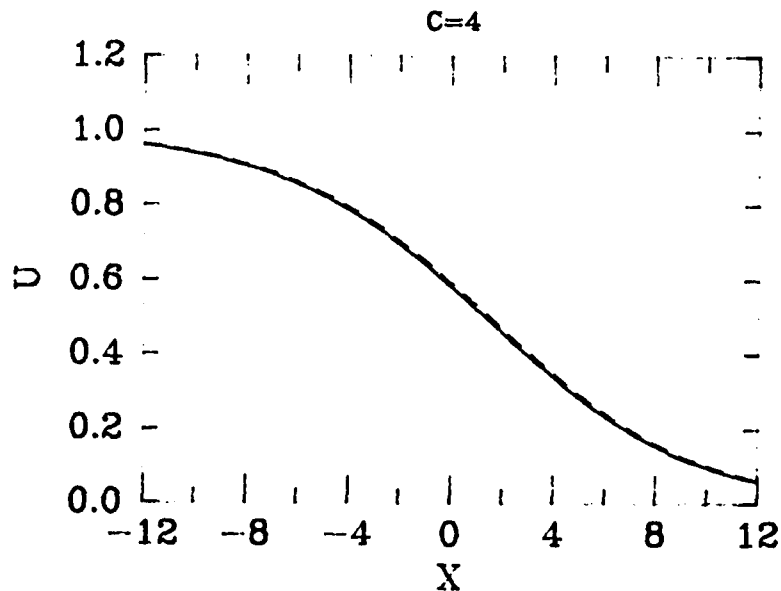


Figure 2

We note that the boundary condition,

$$(3.7) \quad u(\tau_+, t) = \text{constant},$$

leads to good results when the speed of the coordinate system is the same as the speed of the final state. For a more complicated problem, however, this might not be known in advance. Indeed, it might be the goal of the computation to determine it. As shown in Figure 3, our conditions avoid this difficulty. This is the computed evolution in a coordinate system moving with speed 3 of the same initial data used to generate Figure 1. The wave is seen to move to the right and, in fact, moves with relative speed 1. This is confirmed in Figure 4, a comparison of the solution at  $t = 6.875$  (solid line) and the wave of speed 4 of Figure 2 translated to the right a distance of 6.875. We believe the small error at the right boundary is due to the use of linearized boundary conditions.

Figure 5 displays the computed evolution of initial data with two decay rates in the right tail: one compatible with a wave of speed 4, the other compatible with a wave of speed 3. Here, the speed 4 part decayed at the large rate while the speed 3 part decayed at the slow rate. As predicted by the theory, a speed 3 wave is eventually reached.



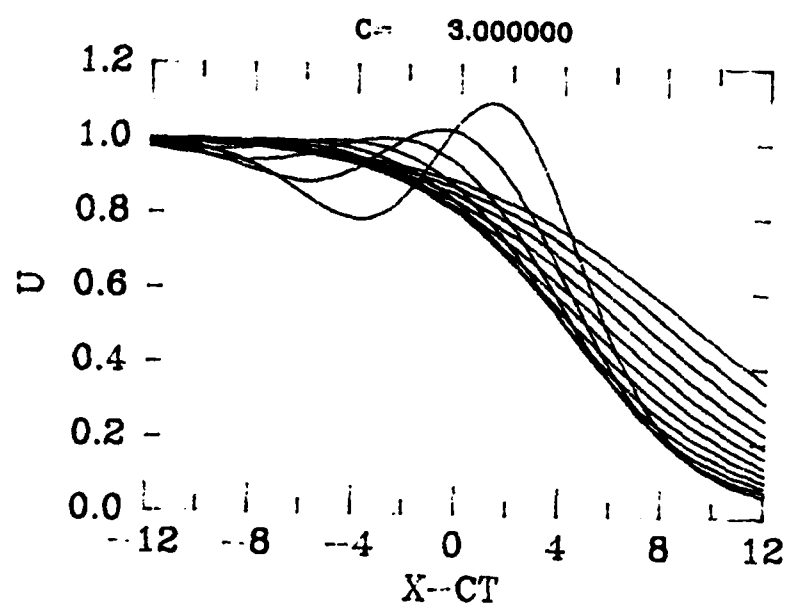


Figure 3

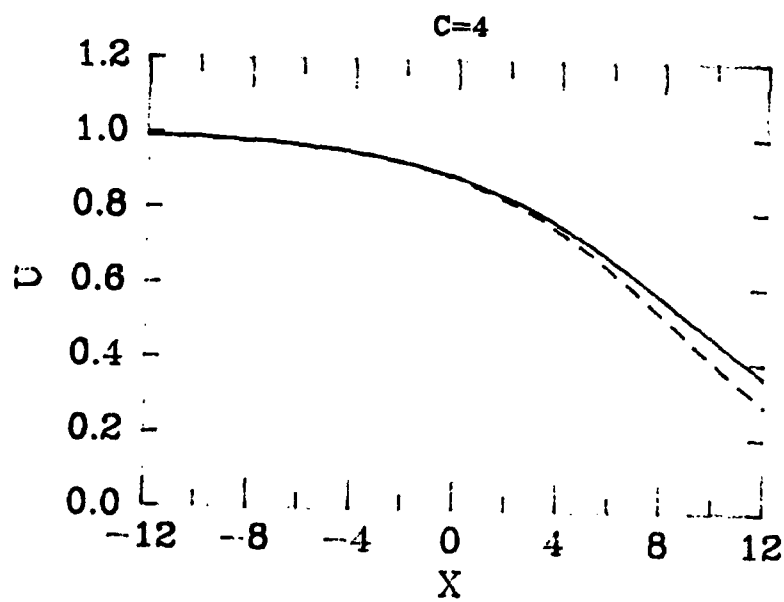


Figure 4

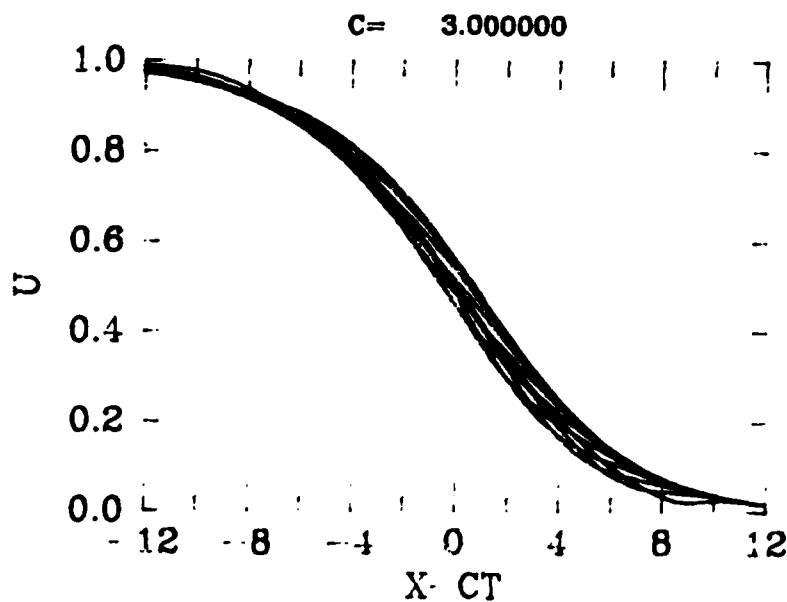


Figure 5

We note that, as it is the initial data in the right tail which determines the wavespeed, it is the right boundary condition which is important. Various choices for the left boundary condition, for example  $u = \text{constant}$  and  $u_x = 0$ , were tried and led to good results.

In summary, we have shown that our boundary conditions consistently lead to correct long time results while other simpler conditions do not. We hope that their generalization to more complicated problems, where the final state is not known a priori, will also give reliable results. It should be noted, however, that this has not been proved even in the simple case described here.

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)  The long time behavior of the solutions of nonlinear parabolic initial value problems on the line has been investigated by many authors. In particular they have shown, under certain assumptions, the existence of traveling waves to which a large class of initial data eventually evolves. They have also proved that which traveling wave solution is picked out as the		

ABSTRACT (cont.)

asymptotic state often depends on the behavior of the initial data at infinity. This causes difficulties for the numerical simulation of the long time evolution of such problems. In particular, if an artificial boundary is introduced, the boundary condition imposed there must depend on the initial data in the discarded region. In this work we derive such boundary conditions, based on the Laplace transform solution of the linearized problems at  $t^\infty$ . We illustrate their utility by presenting a numerical solution of Fisher's equation, a nonlinear parabolic equation with traveling wave solutions which has been proposed as a model in genetics.

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